Binding Affinity of a diimine-dithiolene Ni(II) complex with Bovine Serum Albumin: Spectroscopic and Docking Studies

S. Balou, A. Daflou, M. Vlara, C.A. Mitsopoulou

Inorganic Chemistry Laboratory, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou 15771, Greece

Presenting Author: sbalou@chem.uoa.gr

The interactions between potential drugs and biomolecules are of great importance for the chemists and biologists. Many metal complexes show fascinating results when they interact with DNA, exerting their anticancer activity. Furthermore, Serum albumins (SA) are the most abundant proteins in blood and are responsible for a variety of processes in organisms [1]. The most important physiological function they exhibit is the ability to transport and deliver an amazingly high number of molecules [2]. Therefore, the investigation of interactions between potential medicinal compounds and SA rises as an important aspect in life sciences.

During the last decades, nickel is attracting the interest of the scientific community since it it is one of the essential elements in biological systems [3]. There are many studies of nickel complexes that exhibit antibacterial, antifungal, anticancer and antiproliferative properties [4-6]. In addition, there are numerous planar N-substituted metal complexes that are used as chemical or photochemical probes in nucleic acids. So, the mode of binding of such complexes with SA can reveal the concentration of them in blood and as a consequence the extent of biological action [3], [7].

In our laboratory a synthesized planar nickel complex with diimine and dithiolate ligands was explored for its interaction with BSA. The choice of bovine serum albumin (BSA) from SA is based on its resemblance to the human serum albumin (HAS). The interaction between the aforementioned nickel complex and BSA was examined by spectroscopic methods. Finally, docking studies were able to reveal the binding mode.

References

1. Phopin K, Ruankham W, Prachayasittikul S, Prachayasittikul V, Tantimongcolwat T. International Journal of Molecular Sciences. 21(1) (2020) 249.
2. Topală, T., Bodoki, A., Oprean, L., & Oprean, R. Clujul Medical, 87(4) (2014) 215.
3. Wei, Q., Dong, J., Zhao, P., Li, M., Cheng, F., Kong, J., & Li, L. Journal of Photochemistry and Photobiology B: Biology, 161 (2016) 355–367.
4. N.C. Kasuga, K. Sekino, C. Koumo, N. Shimada, M. Ishikawa, K. Nomiya, Synthesis, structural characterization and antimicrobial activities of 4- and 6-coordinate nickel(II) complexes with three thiosemicarbazones and semicarbazone ligands, J. Inorg. Biochem. 84 (2001) 55–65.
5. M. Alexiou, I. Tsivikas, C.D. Samara, A.A. Pantazaki, P. Trikalitis, N. Lalioti, D.A. Kyriakidis, D.P. Kessissoglou, High nuclearity nickel compounds with three, four or five metal atoms showing antibacterial activity, J. Inorg. Biochem. 93 (2003) 256–264
6. Gao, C.-Y., Ma, Z.-Y., Zhang, Y.-P., Li, S.-T., Gu, W., Liu, X., Yan, S.-P. RSC Advances, 5(39) (2015) 30768–30779.
7. Anjomshoa, M., Torkzadeh-Mahani, M., Sahihi, M., Rizzoli, C., Ansari, M., Janczak, J., Amirheidari, B. Journal of Biomolecular Structure and Dynamics, (2018) 1–51.